Detecting metastable states of dynamical systems by recurrence-based symbolic dynamics

Peter beim Graben[1,2,3,*] and Axel Hutt[3]

[1]*Dept. of German Language and Linguistics, Humboldt-Universität zu Berlin, Germany*

[2]*Bernstein Center for Computational Neuroscience Berlin, Germany*

[3]*Cortex Project, INRIA Nancy Grand Est, France*

(Dated: January 11, 2013)

Abstract

We propose a fast and efficient algorithm for the detection of metastable states of complex dynamical systems from time series. Our approach exploits the characteristic checkerboard texture of metastable states exhibited in recurrence plots (RP). On phase space, RPs induce a reflexive and symmetric, but not transitive, tolerance relation whose transitive closure yields a phase space partition into metastable states. We construct this partition by a rewriting grammar applied to the symbolic dynamics of time indices.

PACS numbers: 89.75.Fb, 05.45.Tp, 05.10.-a, 05.45.-a

The identification of metastable states in complex dynamical systems has become increasingly important in recent time. Its significance ranges from spin glasses [1] and molecular configurations [2] over geoscientific applications [3] to the neurosciences [4–7].

Metastable or quasi-stationary states are regions in the system's phase space with relatively large dwell that are connected by transients [1, 8]. Paradigmatic examples are *almost invariant sets* [9], such as the "wings" of the Lorenz attractor centered around its unstable foci [10], or saddles connected by heteroclinic trajectories [7, 11].

For the identification of metastability in time series, their characteristic slow time scales have been separated from the fast dynamics of phase space trajectories by several clustering algorithms [1, 2, 4, 9, 11, 12]. One method, sometimes called *Perron clustering* [2], starts with some *ad hoc* partitioning of the system's phase space that leads to an approximate Markov chain description [1, 2, 4, 9, 12]. Applying spectral clustering methods to the resulting transition matrix yields the time scales of the process, while their corresponding (left-)eigenvectors allow the unification of cells into a partition of metastable states [4, 12]. Another approach by Hutt et al. [11] utilizes the slowing-down of the system's trajectory in the vicinity of saddles by means of phase space clustering.

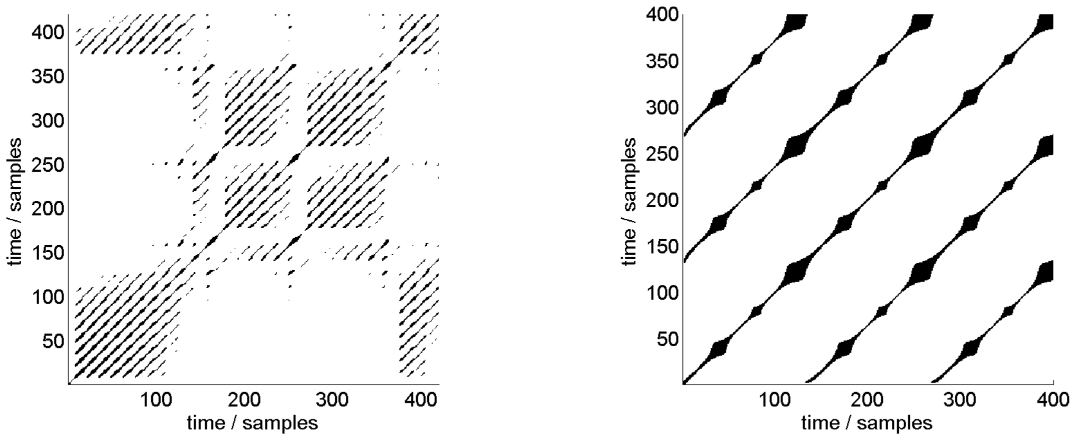
However, those methods might be computationally cumbersome in some applications. In particular, spectral clustering and partitioning could be problematic for higher-dimensional spaces and sparse data, because either the full phase space or a lower-dimensional projection has to be initially partitioned into equally populated cells from which counting measures are to be derived for the estimation of Markov transition matrices [4].

In this Letter, we propose a parsimonious, fast and feasible algorithm for the identification of metastable states in dynamical systems from measured or simulated time series. Our approach is inspired by Poincaré's famous *recurrence theorem* [13]: When $B_\varepsilon(x_0)$ is a "ball" of radius $\varepsilon > 0$ centered at initial condition $x_0 \in X$, where $X \subset \mathbb{R}^d$ denotes the system's phase space of dimension d, then there is an infinite sequence of iterates $x_{t_k} = \Phi^{t_k}(x_0)$ returning to $B_\varepsilon(x_0)$, such that $x_{t_k} \in B_\varepsilon(x_0)$ for all sub-indices $k \in \mathbb{N}$. Here, $\Phi^t : X \to X$ for a given time t describes the system's flow in phase space. These recurrences can be visualized by means of Eckmann et al.'s [14] recurrence plot (RP) method where the element

$$R_{ij} = \Theta(\varepsilon - ||x_j - x_i||) \tag{1}$$

of the *recurrence matrix* $\boldsymbol{R} = (R_{ij})$ is one if $x_j \in B_\varepsilon(x_i)$ and zero otherwise [14, 15], as

mediated by the Heaviside step function Θ. Eckmann et al. [14] have already pointed out that RPs display metastability by a characteristic "checkerboard texture". We illustrate this in Fig. 1 with two paradigmatic RPs for the Lorenz attractor [10] and for a stable heteroclinic contour of three competing Lotka-Volterra populations [7] in Fig. 1(a) and (b), respectively [21].



(a) (b)

Figure 1: Recurrence plots [Eq. (1)] for Euclidian norm of (a) Lorenz attractor and (b) stable heteroclinic contour of a Lotka-Volterra system. Parameters: (a) $\varepsilon = 5$, (b) $\varepsilon = 0.1$. Black pixels denote $R_{ij} = 1$, white ones $R_{ij} = 0$.

Both RPs exhibit the typical texture of diagonal line patters that are characteristic for oscillatory dynamics. For the Lorenz system shown in Fig. 1(a) these oscillators correspond to the metastable wings. Going along the line of identity (LOI) reveals transient transitions between about four metastable states, while the horizontal and vertical recurrences of the same patterns indicate that there are indeed only two metastable states being involved, namely the wings, repeatedly explored by the system's trajectory. On the other hand, the texture of Fig. 1(b) represents a periodic winnerless competition [7, 16] where the characteristic slowing-down in the vicinity of a saddle [11] is reflected by the broadening of horizontal, respective, vertical lines, indicating an increased number of recurrences within an ε-ball around the saddle [15].

For uniform ε, the recurrence matrices obtained from Eq. (1) are reflexive, $R_{ii} = 1$ (the LOI), and symmetric, $R_{ij} = R_{ji}$, but in general not transitive, i.e. $R_{ij} = 1$ and $R_{jk} = 1$ do not necessarily imply $R_{ik} = 1$. In order to cope with this disadvantage, Faure and Lesne

[17] suggested to compute the recurrence matrix from words in a symbolic dynamics [18] through

$$R^+_{ij} = \delta_{w_i w_j} \, , \tag{2}$$

where w_i, w_j are words of length m at times i and j in a symbolic sequence $s = a_1 a_2 \dots a_n$. Here, $\delta_{ab} = 1$ if $a = b$ and zero otherwise, denotes the Kronecker matrix. Symbolic RPs given by Eq. (2) are also transitive, because symbolic dynamics results from a partition of the system's phase space into equivalence classes.

However, for the more general case of ε-RPs [Eq. (1)], we can still define a *tolerance relation* xRy [19] on phase space X as follows: we say $x \in X$ R-tolerates $y \in X$, xRy, if there exists an initial condition $x_0 \in X$ and a time t such that (1) $x \in B_\varepsilon(x_0)$, (2) $y \in B_\varepsilon(x_t)$ and (3) $x_t \in B_\varepsilon(x_0)$, i.e. $R_{0t} = 1$. Here, $x_t = \Phi^t(x_0)$ is again the iterate of x_0. The tolerance relation R is reflexive: xRx, since $R_{00} = 1$; it is symmetric: xRy implies yRx as $R_{0t} = R_{t0}$; but it is not transitive: xRy and yRz do not imply xRz

Nevertheless, we can construct the *transitive closure*, R^+, of R which is possible for every relation. This new relation would be an equivalence relation whose equivalence classes partition the phase space into unions of recurrent and thus intersecting ε-balls which cover the metastable states. We achieve this construction by regarding the ε-RP $\boldsymbol{R}$ [Eq. (1)] as a *grammatical rewriting system* over the time indices of a given trajectory x_t [20]. Thus, we first map the trajectory x_t to the sequence of successive time indices, regarded as symbols: $x_t \to s_t = t$. Then we define a formal grammar of rewriting rules: if $i > j$ and $R_{ij} = 1$ create a rule $i \to j$. To enforce transitivity for $i > j > k$, $R_{ij} = 1$ and $R_{ik} = 1$, we first eliminate the redundancy by rewriting only $i \to k$ and then create an additional rule $j \to k$. Finally, we apply this grammar to the initial sequence of time indices $s_t = t$ in order to replace large indices by smaller ones, thus exploiting the recurrence structure of the data. The result is a transformed symbolic sequence s'_t, whose symbolic RP $\boldsymbol{R}^+$ [Eq. (2)] [17] yields the transitive closure R^+ of the tolerance relation R on phase space.

As R^+ is an equivalence relation, its equivalence classes partition the phase space into metastable states. This partition contains the union of intersecting ε-balls along the sampled trajectory together with its complements.

Let us illustrate the procedure by means of a simple example. Assume, we have a series

of only five data points $(x_1, x_2, \ldots, x_5)$ that gave rise to the recurrence matrix

$$\boldsymbol{R} = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{bmatrix} \tag{3}$$

The algorithm starts in the 5th row, detecting a recurrence $R_{52} = 1$. Since $5 > 2$, we create a rewriting rule $5 \to 2$. Because the next recurrence in row 5 is trivial, the algorithm continues with row 4, where $R_{41} = R_{42} = 1$. Now, two rules $4 \to 1$ and $4 \to 2$ could be generated. However, the latter is redundant. Therefore the algorithm only records the rule $4 \to 1$. Moreover, transitivity is taken into account by an additional rule $2 \to 1$. Next, row 3 does not contribute to the algorithm and rows 2 and 1 can be neglected due to the symmetry. Recursively applying this grammar to the symbolically encoded time series $s = \ll 12345 \gg$ yields $s' = \ll 11311 \gg$, i.e. a bistable system with states $\ll 1 \gg$ and $\ll 3 \gg$.

In order to validate our construction, we employ the method to the examples from Fig. 1. Yet, for the ball size ε chosen in Fig. 1, every phase space point turns out to be equivalent to every other point, leading to a trivial partition. We therefore diminish ε in such a way that the resulting ε-RPs become too sparse for visualization. Furthermore, we find a tradeoff between ε and the sampling rate. When the latter is too small, metastable states could be reflected by spurious oscillations in the symbolic dynamics s'_t. Thus, we also increased the sampling rate for the Lorenz attractor and the Lotka-Volterra system.

Figure 2 shows the three time series $x_1(t), x_2(t), x_3(t)$ from the numeric solution of the Lorenz attractor (a) and of the heteroclinic contour in the Lotka-Volterra populations (b), together with the suitably rescaled symbolic sequence s' obtained from our recurrence-based partitioning method.

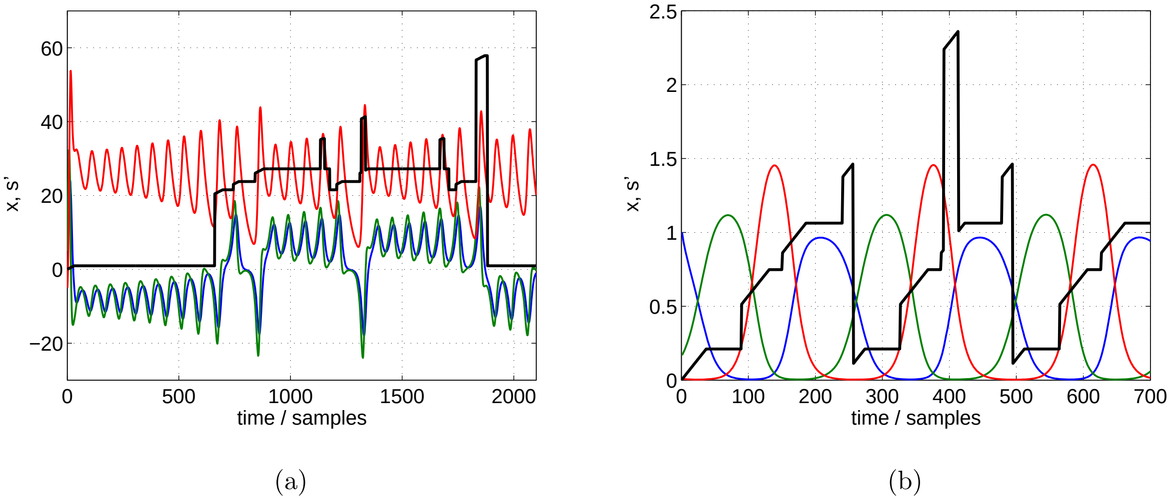


Figure 2: (Color online) Time series of (a) Lorenz attractor and (b) stable heteroclinic contour of a Lotka-Volterra system. Blue: $x_1(t)$, green: $x_2(t)$, red: $x_3(t)$. The black curve displays the (rescaled) symbolic sequence $s'(t)$ from the recurrence-based phase space partition. Parameters: (a) $\varepsilon = 1$, (b) $\varepsilon = 0.013$.

In Fig. 2(a) the switching from one metastable state, i.e., wing, into another one is simultaneously reflected by the sign change of coordinates x_1, x_2 and by the jumps between the long-lasting plateaus of the symbolic dynamics s'. Short transients between metastable states are represented by monotonically increasing pieces of s'. This is even more salient in Fig. 2(b), where most of the heteroclinic dynamics is transient. On the other hand, the characteristic slowing down in the vicinity of the saddles leads to increased recurrences and hence to the plateaus in s', again.

Figure 3 displays the symbolic recurrence plots Eq. (2) of s' for word length $m = 1$, $\boldsymbol{R}^+$, as the transitive closure R^+ of the tolerance relation R.

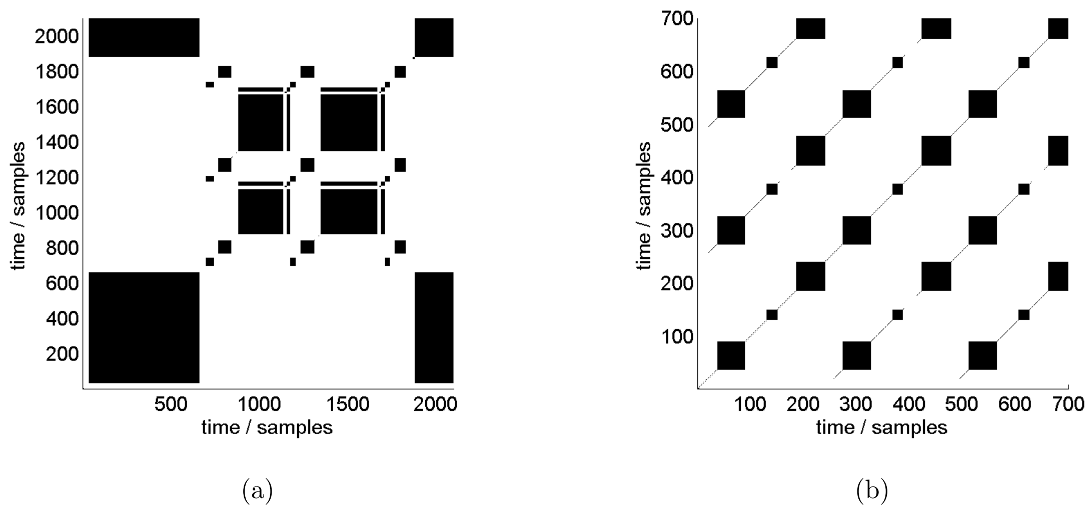
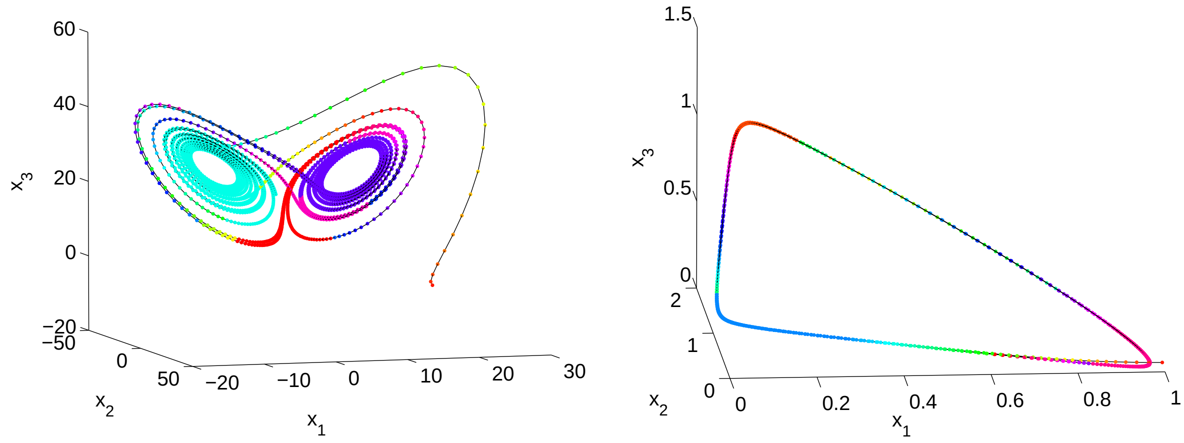


Figure 3: Symbolic recurrence plots [Eq. (2)] of (a) Lorenz attractor and (b) stable heteroclinic contour of a Lotka-Volterra system. Black pixels denote $R^+_{ij} = 1$, white ones $R^+_{ij} = 0$.

After the recurrence-based symbolic encoding, the checkerboard texture indicating the metastable states is highly enhanced for the Lorenz attractor Fig. 3(a) in comparison to Fig. 1(a) and for the Lotka-Volterra system Fig. 3(b) compared with Fig. 1(b).

Finally, we combine the phase space information contained in the state vector $x \in X$ with that contained in the symbolic dynamics s' at one instance of time t for identifying metastable states in phase space.

Figure 4 depicts the trajectories around the Lorenz attractor (a) and around the heteroclinic contour (b) where each sampled state x_t at time t is colored according to the symbol s'_t using a rotating color palette.



(a) (b)

Figure 4: (Color online) Phase space partitions into metastable states obtained from recurrence-based symbolic dynamics. (a) Lorenz attractor and (b) stable heteroclinic contour of a Lotka-Volterra system. Colored balls indicate the membership to a partition cell.

Now, transients are represented by continuously changing colors while metastable states are homogeneously colored regions in phase space. For the Lorenz attractor in Fig. 4(a) these are the wings essentially colored in turquoise and dark blue. For the Lotka-Volterra dynamics in Fig. 4(b) the metastable states are the vertices of the "triangle" colored in blue, red and purple.

In this Letter we proposed a parsimonious, fast and feasible algorithm for the detection of metastable states in complex dynamical systems. In contrast to techniques based on Markov chains, which require an *ad hoc* partitioning of the system's phase space into equally populated cells, the estimation of transition probabilities by counting measures and subsequent spectral clustering methods, our approach simply exploits the recurrence structure of the system's dynamics by taking the transitive closure of the recurrence plot, thereby partitioning the phase space into unions of intersecting ε-balls along the actual trajectory.

The proposed method could have a number of interesting applications in many different fields, such as molecular dynamics [2], geo- [3], and neurosciences [4–7] for the identification of metastable behavior. Moreover, it could also be useful for the analysis of complex networks for solving graph partition and related problems by taking the transitive closure of the graph's adjacency matrix.

This research has been supported by the European Union's Seventh Framework Pro-

gramme (FP7/2007-2013) ERC grant agreement No. 257253 awarded to AH, hosting PbG during fall 2012 in Nancy, and by a Heisenberg fellowship (GR 3711/1-1) of the German Research Foundation (DFG) awarded to PbG. We thank Pedro Ernesto Garcia-Rodriguez, Slawomir Nasuto and Harald Atmanspacher for stimulating discussions.

---

* Electronic address: peter.beim.graben@hu-berlin.de

[1] H. Larralde and F. Leyvraz, Physical Review Letters **94**, 160201 (2005).

[2] P. Deuflhard and M. Weber, Linear Algebra and its Applications **398**, 161 (2005).

[3] G. Froyland, K. Padberg, M. H. England, and A. M. Treguier, Physical Review Letters **98**, 224503 (2007).

[4] C. Allefeld, H. Atmanspacher, and J. Wackermann, Chaos **19**, 015102 (2009).

[5] K. J. Friston, NeuroImage **5**, 164 (1997).

[6] M. I. Rabinovich, R. Huerta, and G. Laurent, Science **321**, 48 (2008).

[7] M. I. Rabinovich, R. Huerta, P. Varona, and V. S. Afraimovich, PLoS Computational Biology **4**, e1000072 (2008).

[8] C. G. Tokman, B. R. Hunt, and P. Wright, Ergodic Theory and Dynamical Systems **31**, 1345 (2011).

[9] G. Froyland, Physica D **200**, 205 (2005).

[10] E. N. Lorenz, Journal of the Atmospheric Sciences **20**, 130 (1963).

[11] A. Hutt and H. Riedel, Physica D **177**, 203 (2003).

[12] B. Gaveau and L. S. Schulman, Physical Reviews E **73**, 036124 (2006).

[13] H. Poincaré, Acta Mathematica **13**, 1 (1890).

[14] J.-P. Eckmann, S. O. Kamphorst, and D. Ruelle, Europhysics Letters **4**, 973 (1987).

[15] N. Marwan and J. Kurths, Physics Letters **A 336**, 349 (2005).

[16] M. Rabinovich, A. Volkovskii, P. Lecanda, R. Huerta, H. D. I. Abarbanel, and G. Laurent, Physical Review Letters **87**, 068102 (2001).

[17] P. Faure and A. Lesne, International Journal of Bifurcation and Chaos **20**, 1731 (2010).

[18] B.-L. Hao, *Elementary Symbolic Dynamics and Chaos in Dissipative Systems* (World Scientific, Singapore, 1989).

[19] Y. A. Shreider, Cybernetics **6**, 153 (1970).

[20] J. E. Hopcroft and J. D. Ullman, *Introduction to Automata Theory, Languages, and Computation* (Addison–Wesley, Menlo Park, California, 1979).

[21] See Supplementary Material for numeric implementation details.